

1,4-Diazabicyclo[2.2.2]octane
280-57-9 | DTXSID0022016

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.85	1.14	0.85	1.12	0.83	1.23

Model Results

Predicted value: 1.30×10^{-11} cm³/molecule*sec

Global applicability domain: Inside

Local applicability domain index: 8.23×10^{-1}

Confidence level: 7.77×10^{-1}

Nearest Neighbors from the Training Set

Image not found

1,4-Diazabicyclo[2.2.2]octane

Measured: 2.20×10^{-11}

Predicted: 1.30×10^{-11}

Image not found

2-Butanol

Measured: 9.60×10^{-12}

Predicted: 8.64×10^{-12}

Image not found

1-Butanol

Measured: 8.57×10^{-12}

Predicted: 1.06×10^{-11}

Image not found

Cyclopentanol

Measured: 1.07×10^{-11}

Predicted: 1.17×10^{-11}

Image not found

1-Propanol

Measured: 5.53×10^{-12}

Predicted: 7.35×10^{-12}